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Overview of models used in land treatment of wastewater

I.K. Iskandar

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This report summarizes the state of the art of the modeling of wastewater renovation by land treatment. The models discussed are classified based on their use for planning, site selection and cost analysis, and for predicting 1) water and salt transport in soils, 2) nitrogen transport and transformations, 3) phosphorus transport and transformations, 4) virus movement in soils, and 5) toxic metal and trace organic movement in soils. This report compares the different models as to their purpose, input and output data, and status of validation. In addition, the report includes a section on research needs for modeling land treatment of wastewater.

PREFACE

This report was prepared by Dr. I.K. Iskandar, Research Chemist, of the Earth Sciences Branch, Research Division, U.S. Army Cold Regions Research and Engineering Laboratory. This study was conducted under Civil Works Projects CWIS 31633, Optimization of Automated Procedures for Planning, Design and Management of Land Treatment Systems and CWIS 31732, Land Treatment Management and Operation.

This report was technically reviewed by S. Reed (CRREL), Dr. C. Enfield (EPA - Ada, Oklahoma), Dr. M.B. Kirkham (Kansas State University), Dr. W.W. Huang (EPA, Washington, D.C.), Dr. R. Smith (University of California, Davis), and W. Opfer (Agricultural Research Service, Washington, D.C.).

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by

I.K. Iskandar

INTRODUCTION

During the past few years interest has been increasing in developing mathematical models to simulate complex biological processes in the environment. Many models have been developed specifically for land treatment or can be adapted for use with land treatment systems.

The purpose of this report is to present an overview of the use of such models for land treatment planning, design and operation. Detailed examination of some of these models and their status of evaluation have been presented elsewhere (Frissel and van Veen 1981, Iskandar 1981). Emphasis is placed here on the type and availability of models, processes described, input and output data and the purpose of model development.

TYPES OF MODELS

In general, there are two approaches to modeling: simulation modeling and optimization modeling. Simulation modeling is an attempt to describe the behavior of a system without actually using the physical system or its prototype. Optimization modeling, on the other hand, is usually used to improve the decision-making process by the use of mathematics. Simulation models may be further divided into other types, such as deterministic, compartmental and stochastic. A deterministic model computes the outcome of an activity that can be completely described in terms of input and processes involved thereafter. In compartmental models, the complex system is divided into subcompartments or blocks primarily to simplify different simultaneous processes or interactions that take place in the system. A stochastic model is based on statistical relationships rather than mechanisms involved.

Simulation models can also be divided into lumped and distributed parameter models. A lumped parameter model examines the input-output relationships as a function of time but not of space. In contrast, the distributed parameter model considers the internal spatial units, each of which

is separately examined. Therefore, the model describes input-output as a function of both time and space. Lumped parameter models that are highly aggregated are called "black-box" models. Other frequently used adjectives for models are "empirical" vs. "mechanistic," "steady-state" vs. "dynamic," "equilibrium" vs. "rate," "analytic" vs. "numeric," and so forth (Tanji 1981).

MODELS FOR PLANNING, SITE SELECTION AND COST ANALYSIS

For land treatment planning, site selection and cost analysis, several rational procedures and models are available (Spaine and Merry 1978, Young 1978, Bouma 1981 and Lynch and Kirshen 1981).

Bouma (1981) discussed simple procedures for using soil survey data with the help of computer simulation mapping in preliminary planning and site selection of land treatment systems. Soil survey reports as executed by the National Cooperative Soil Survey Program of the U.S. Department of Agriculture's Soil Conservation Service (Soil Survey Staff 1951, 1975) contain two types of data: 1) data that have direct relevance to system design, such as the slope of the land, depth of groundwater, and measured soil, chemical and physical properties, and 2) data that can be used indirectly to estimate relevant soil properties, such as soil texture and organic matter content. These data may be used to predict soil structure and preferential flow patterns. For example, Bouma (1981) gives a method of predicting the moisture content (θ) of surface soils at a given moisture tension (s), organic matter content (OM) and dry bulk density (ρ) with the following relationship:

$$\theta = 34 - 0.339\ OM + 0.23\ s + 78.15\ \rho. \qquad (1)$$

For a given soil, OM and ρ do not change significantly over a short period of time, while θ and s are always in a dynamic condition.

This simple equation would be useful in establishing irrigation schedules for land treatment systems. Moisture retention curves could be determined in the laboratory, and hence the water content of the soil as a function of time could be calculated.

For regional planning and site selection, Bouma (1981) and Moser (1978) showed how to use the soil survey information and health code criteria to classify soils as to their suitability for waste disposal and treatment. Soils were classified as having slight, severe and very severe limitations. The method developed By Moser (1978) was used during the

feasibility study of land treatment in the Nashville metropolitan region (Metcalf and Eddy 1978).

Optimization models may be used for land treatment planning, design, crop selection and in land treatment management and operation in general. Lynch and Kirshen (1981) used linear programming techniques to illustrate the use of two such models with hypothetical examples based on published data. Their first model provides information on when wastewater should be applied and which crop should be grown during each season, so that groundwater quality can be maintained and costs minimized. The second model, designed to be used after the first model has been solved, determines the detailed weekly application rate of wastewater and nutrients for each crop through a single growing season. The land area devoted to each crop and the levels of wastewater storage both at the beginning and end of the growing season are taken from the results of the first model. Baron (1981) and Baron et al. (1982a,b) reviewed the literature on the use of optimization models as tools for planning, design and operation of land treatment in cold climates and developed a model using nonlinear programming for optimum design of slow rate systems, including lagoon pretreatment alternatives.

The computer model CAPDET (Computer Assisted Procedure for the Design and Evaluation of Wastewater Treatment Systems) was developed in 1972 to complement a Corps of Engineers design manual on wastewater management (U.S. Department of the Army 1972) and was updated to include cost analysis for land treatment alternatives (Spaine and Merry 1978). In the revised version of CAPDET are five basic land treatment alternatives: rapid infiltration, overland flow, slow rate, ridge and furrow irrigation, and flood irrigation. Inputs to the model are application rate, width of buffer zone (if any), application period, wastewater generation period, cost of land, storage period, cost of site preparation, cost of distribution pumping and recovery system, and wastewater characteristics. The outputs from CAPDET include total land requirements, mean percolate water quality, required capital, and operation and maintenance costs of wastewater renovation.

In general CAPDET and other cost models, such as that developed by Young (1978), can be used as tools for preliminary planning and site selection of land treatment.

Table 1. Review of available salt and water flow models (from Gupta et al. 1978).

Authors/year*	Water flow model: Type of flow		Water flow model: Initial conditions				Water flow model: Boundary conditions					Salt flow model: Type of flow			Salt flow model: Initial Conditions		Salt flow model: Sink or source		Salt flow model: Exchange reactions				Salt flow model: Precipitation & solubilization				Validation	
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
Analytical Solutions																												
Wilson (1940)	x		x	x	x		x					x			x			x	x								
DeVault (1943)	x		x	x	x		x					x			x			x	x								
Glueckauf (1949)	x		x	x	x		x					x			x			x									
Lapidus & Amundson (1952)	x		x	x	x		x					x	x		x			x									
Ribble & Davis (1955)	x		x		x		x					x			x			x	x	x	x					x	
Molen (1956)	x			x	x		x					x			x		x										x
Bower et al. (1957)	x		x	x	x		x					x			x			x	x	x	x					x	
Gardner & Brooks (1957)	x		x	x	x		x					x			x			x	x	x	x					x	
Nielson & Biggar (1962)	x		x	x	x		x					x	x		x		x									x	
Biggar & Neilsen (1963)	x		x	x			x					x					x	x	x							x	
Elrick et al. (1966)	x		x	x	x		x					x	x	x	x		x	x							x	x	
Cho (1971)	x		x	x	x		x					x	x		x		x	x							x		
Misra et al. (1974)	x		x	x	x		x					x	x		x		x	x							x	x	
Skopp & Warrick (1974)	x		x	x	x		x					x	x		x			x		x							
Cassel et al. (1975)	x		x	x	x		x					x	x		x		x									x	
van Genuchten & Wierenga (1976)	x		x	x	x		x					x	x	x	x		x	x									
Numerical Solutions																												
Bresler (1967)	x			x		x	x					x				x	x										x
Bresler & Hanks (1969)	x	x	x	x		x	x	x	x		x	x				x	x									x	
Lai & Jurinak (1971)	x			x	x		x					x	x		x			x	x	x	x	x				x	
Warrick et al. (1971)	x	x	x	x		x	x					x	x				x										x
Dutt et al. (1972)	x	x	x	x		x	x	x	x	x	x	x				x	x	x	x	x	x	x	x	x	x	x	x	
Gupta (1972)	x	x	x	x		x	x	x	x	x	x	x				x	x	x	x	x	x	x	x	x	x		x	x
Bresler (1973)	x	x	x	x		x	x	x	x		x	x	x	x													x	x
Kirda et al. (1973)	x	x	x	x		x	x	x				x	x			x	x									x	
Shaffer et al. (1977)	x	x	x	x		x	x	x	x	x	x	x	x			x	x	x	x	x	x	x	x	x	x	x	x	x
Selim & Iskandar (1981)	x	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x	x	x							x	x	x

* For complete citations, see Gupta et al. 1978 (except for Selim and Iskandar 1981, which is given in the Literature Cited)

1. Steady
2. Transient
3. Saturated
4. Unsaturated
5. Uniform initial water content
6. Variable initial water content
7. Infiltration
8. Redistribution
9. Evaporation
10. Transpiration
11. Water table
12. Convective flow
13. Molecular diffusion
14. Hydrodynamic dispersion
15. Uniform initial salt concentration
16. Variable initial salt concentration
17. Non-interacting solutes
18. Interacting solutes
19. Exchange reaction considered
20. Ca-Mg
21. Ca-Na
22. Mg-Na
23. $CaSO_4$
24. $CaCO_3$
25. Ca, Mg, SO_4, ion pair
26. Nitrogen transformation
27. Laboratory
28. Field

MODELS FOR PREDICTING WATER AND SALT TRANSPORT IN SOILS

Research-oriented models

The type of transport model most commonly used to simulate water and salt movement is the convective-diffusion model. Soil water flow in the presence of a transpiring crop may be described (see Selim 1978) by

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta)\frac{\partial \theta}{\partial z} - k(\theta)\right] - W(z,t) \qquad (2)$$

where θ is the volumetric water content, t time, z the space coordinate, D the soil-water diffusivity, k the hydraulic conductivity, and W the root water extraction.

The transport of reactive solute species may be described (Tanji 1981) by

$$\frac{\partial(\theta C_i)}{\partial t} = \frac{\partial}{\partial z}\left[D(v,\theta)\frac{\partial C_i}{\partial z}\right] - \frac{\partial}{\partial z}\left(q\frac{C_i}{\partial z}\right) - \frac{\partial(\rho s)}{\partial t} \pm \phi_i \qquad (3)$$

where C_i is the concentration of the solute species i, D the apparent diffusion coefficient of the solute species, v the average pore-water velocity, q the volumetric water flux, ρ the soil bulk density, s the adsorbed solute species, and ϕ_i the sink/source term for C_i. For a nonreactive solute species the term $\partial(\rho s)/\partial t$ drops out.

Inputs to the water and salt transport models include data on soil physical properties, such as hydraulic conductivity and diffusivity, soil depth and slope, depth to groundwater, potential evapotranspiration, plant uptake and sorption-desorption coefficients. Outputs from these models include water and salt distribution in the soil with time and space.

Gupta et al. (1978) reviewed water and salt models and their findings are summarized in Table 1. Of the 26 models reviewed, 16 models used the analytical solution technique for model solving. Most of the models were developed for steady-state conditions and only 8 models included both steady-state and transient conditions.

Application of such models is usually limited to laboratory columns or lysimeters but some models (Addiscott 1981, Enfield 1981 and Shaffer and Gupta 1981) have been used to predict water and solute transport under field conditions. The main difficulty in applying such models to field conditions is the inherent variability of soil characteristics (Bouma 1981, Nielsen et al. 1981a, 1981b). Data on the natural variability of many

physical parameters of soils are lacking but this problem has received much attention in recent years.

Management-oriented models

Several types of management-oriented models have been used to describe a process or processes in land treatment systems. Examples of these models include compartmental models (Mehran et al. 1981), ecosystem models (Riggan and Cole 1981) and conceptual models (Ryden et al. 1981).

The goals and approaches of these models are quite different from those of research-oriented models. However, some of the research-oriented models (Selim and Iskandar 1981, Shaffer and Gupta 1981) have been used for decision-making purposes, and a few of the management-oriented models have contributed to further understanding of interactive processes.

Figure 1 shows a schematic representation of the compartmental water flow model developed by Mehran et al. (1981). By knowing the amounts of wastewater applied (or that can be applied), evapotranspiration, and soil water, one can calculate the leaching losses. The following relations define the unknowns in terms of known quantities:

$$Q_{sw} = e_{iae}\, Q_{iw} + (1 - a)\, Q_p \qquad (4)$$

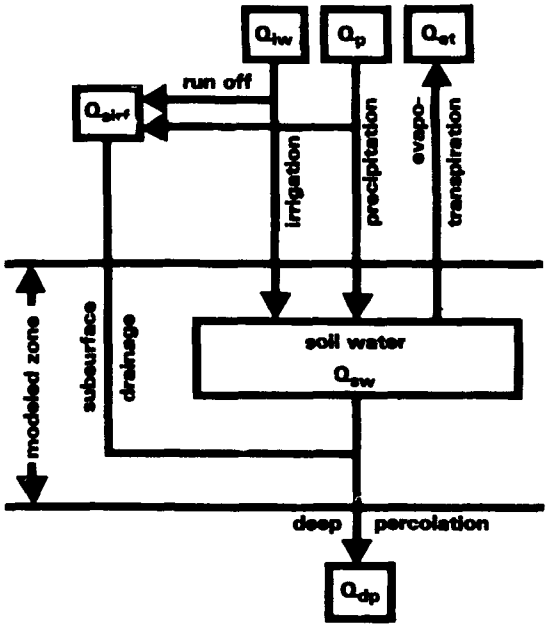

Figure 1. Schematic diagram of water flow submodel (Mehran et al. 1981).

$$Q_{11} = Q_{sw} - Q_{et} \quad (5)$$

$$Q_{dp} = f\ Q_{11} \quad (6)$$

$$Q_{sirf} = (1 - e_{iae}\ Q_{iw}) + a\ Q_p\ (1 - f)\ Q_{11} \quad (7)$$

where a = runoff coefficient

e = crop evapotranspiration coefficient

e_{iae} = irrigation application efficiency

Q_{11} = leaching losses

Q_{sw} = soil water

Q_{iw} = irrigation water

Q_p = precipitation

Q_{et} = evapotranspiration

Q_{dp} = deep percolation

Q_{sirf} = surface irrigation return flow

f = deep percolation coefficient.

All water fluxes are in units of centimeters per year. Besides the known quantities mentioned above, three coefficients must be determined or estimated before the above equations can be solved. These are irrigation application efficiency (e_{iae}), precipitation runoff (a), and the deep percolation coefficient (f). Knowing all these input data and coefficients will allow the calculation of the leaching losses.

This model has been tested with field data from Davis, California, and data from a prototype slow rate system in Hanover, New Hampshire (Mehran et al. 1981). Reasonably good agreement between model predictions and field data were obtained on a mass balance basis.

MODELS FOR PREDICTING NITROGEN TRANSPORT AND TRANSFORMATION

Modeling nitrogen transport and transformations in soil has received the attention of many investigators. Due to the many transformation processes that take place simultaneously (Fig. 2), it is difficult to estimate the fate of N in soils at a specified time and depth. Mathematical models have been used for both quantitative and qualitative understanding and management of N in land treatment systems. Most of these models are kinetic and must be matched with soil water flow models.

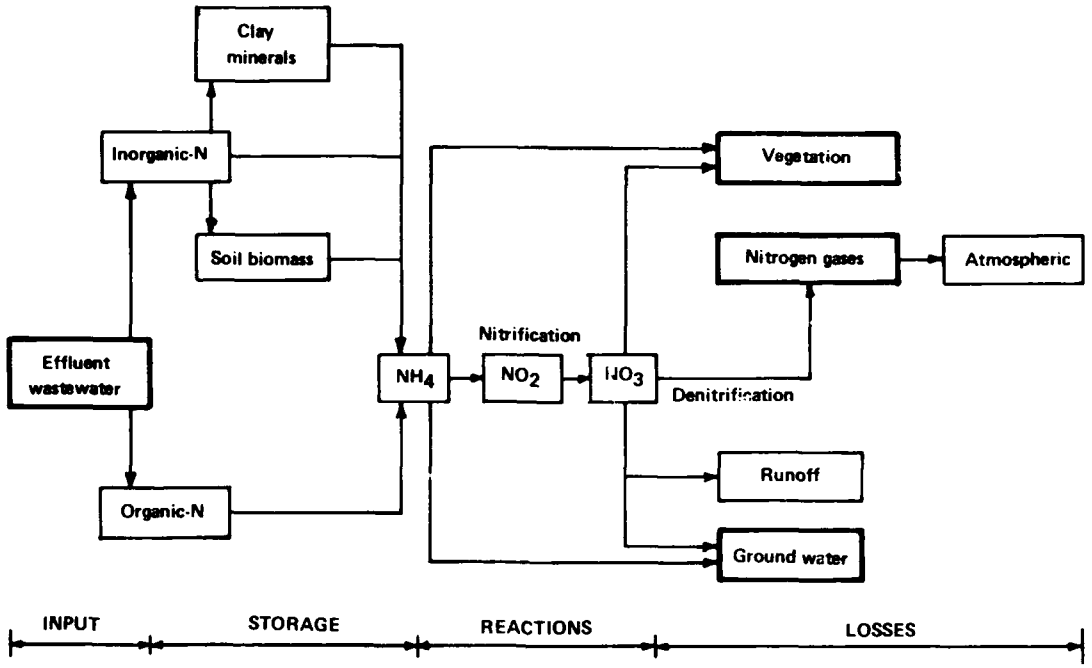

Figure 2. Nitrogen transformation in land treatment.

Modeling the nitrification process

Three types of mathematical models have been used to describe the nitrification process. These models are based on (1) Monod (Michaelis-Menten) kinetics, (2) chemical kinetics, and (3) empirical equations. The Monod kinetic model can be represented by

$$-\frac{\partial[s]}{dt} = \frac{1}{y} \cdot \frac{\partial G}{\partial t} \tag{8}$$

where s is the substrate (NH_4 or NO_2) concentration, t time, G biomass, and y the yield coefficient. The increase in growth (∂G) is obtained from

$$\frac{\partial G}{dt} = \mu G \tag{9}$$

where μ is the specific growth rate, which can be obtained from

$$\mu = \mu_m \frac{[s]}{(K_s + [s])} \tag{10}$$

where μ_m is the maximum specific growth rate and K_s the half saturation constant. Leggett and Iskandar (1980) reviewed the literature on modeling the nitrification process and summarized data for rate constants. Assuming that G and y remain constant, eq 8, 9, and 10 above will be reduced to

$$-\frac{\partial[s]}{dt} = \frac{1}{y} u_m \cdot \frac{[s]}{(K_s + [s])} \cdot G \,. \qquad (11)$$

Examples of the biochemical approach are those of Leggett and Iskandar (1980) and Frissel and van Veen (1981).

The chemical modeling of the nitrification process has been either zero-order kinetic or first-order kinetic as follows:

$$-\frac{d[s]}{\partial t} = k_0 \qquad (12)$$

$$-\frac{d[s]}{\partial t} = k_1(s) \qquad (13)$$

where k_0 and k_1 are the zero and first order reaction rate constants respectively. Examples of the chemical modeling approach are given by Selim and Iskandar (1978), Cho (1971), and Misra et al. (1974).

Empirical equations have often been used when cause-and-effect relationships are not known or when there is an advantage in fitting a model to site-specific experimental data (Parker et al. 1981).

In the chemical model, the rate constants such as k_1 in eq 13 have values over a restricted range. The rate of reaction $\partial[s]/\partial t$, however, may vary widely because of [s] or environmental factors. To include the effect of environmental factors such as temperature, pH, and oxygen content, an empirical factor (f) has been included in the chemical model (Selim and Iskandar 1981):

$$\frac{\partial[s]}{\partial t} = f\ K_1 \qquad (14)$$

where f is a reduction factor ranging from 0 to 1, and K_1 is the maximum rate of nitrification under optimum conditions.

The Monod (Michaelis-Menten) kinetic models are theoretically sound and more complete than the others since they are linked to microbial biomass and enzyme substrate kinetics (Leggett and Iskandar 1980). Such models have the capability of describing the entire time course of change including the lag time. However, they require several input data that are not commonly measured in the field, and it is difficult to measure or validate microbial biomass.

Modeling the denitrification process

Unlike nitrification, denitrification is carried out by a diverse population of aerobic microorganisms (facultative anaerobes) that mediate

NO_3^- reduction under certain O_2-limited conditions and in the presence of soluble (biodegradable) organic carbon as an energy source. Mathematical modeling approaches for denitrification in soils are similar to those for nitrification, including biomass-based kinetics, chemical kinetics and empirical equations. Modeling denitrification, however, requires knowledge of when and where the anoxic conditions prevail. Also, the effects of environmental factors are less defined due to the diverse nature of denitrifying organisms.

The Monod kinetic approach may consist of single (eq 15) or double (eq 16) Michaelis-Menten kinetic model:

$$\frac{\partial[NO_3]}{\partial t} = K_d \frac{[NO_3]}{K_{NO_3} + [NO_3]} \tag{15}$$

$$\frac{\partial[NO_3]}{\partial t} = K_c \frac{[NO_3]}{K_{NO_3} + [NO_3]} \cdot \frac{[\text{soluble organic C}]}{K_{solC} + [\text{soluble organic C}]} \tag{16}$$

where K_d and K_c are the maximum denitrification rates, and K_{NO_3} and K_{solC} are the half-saturation constants for nitrate and soluble or biodegradable carbon respectively.

Chemical kinetics have also been used to describe the denitrification process in soils (Mehran and Tanji 1974, Rao et al. 1981, Selim and Iskandar 1981, Kruh and Segal 1981). However, it is difficult to use first- or zero-order kinetics with respect to NO_3, which varies from 0.08 ppm N (for liquid cultures) to 40 ppm N (in soil). Selim and Iskandar (1981) restricted their study of denitrification to anoxic conditions that prevail when the water content is 80% or greater than the saturation capacity of the soil. Modeling denitrification by either the biological approach or chemical kinetics is hampered by the lack of quantitative estimation of the biodegradable carbon in soils. Empirical models have been used mainly for rapid infiltration systems. In this application, the amounts of N denitrified were assumed to be equivalent to 50% of the biodegradable carbon applied to soils (U.S. Environmental Protection Agency et al. 1981).

Modeling the mineralization-immobilization processes

Modeling of N mineralization and immobilization processes is also largely determined by the great diversity of the microorganisms involved and the effect of environmental factors. These processes occur over a wide range of temperature, pH, and moisture content, and under both aerobic and

anaerobic conditions. An important aspect of the mineralization-immobilization processes is the strong relationship between the soil carbon and nitrogen cycles.

There are three modeling approaches that have been used to simulate these processes:

1. Models which do not consider the carbon decomposition and predict the mineralization of N using first-order kinetics (Tanji and Gupta 1978) or a pseudo-Arrhenius equation (Addiscott 1981).
2. Models which consider carbon and nitrogen and include the C/N ratio as the parameter determining whether or not mineralization or immobilization occurs.
3. Models which consider carbon and nitrogen as substrates for the biomass (Juma and Paul 1981, van Veen and Frissel 1981).

Modeling plant uptake of nitrogen

Nutrient uptake by plants growing in soil depends on the nutrient uptake characteristics of the plant-root system and on the nutrient supply characteristics of the soil. Miller and Stuart (1978) reviewed the state of the art of modeling plant uptake of nutrients and concluded that plant uptake models vary greatly in their objectives and in the processes included. They suggested that a combination of several parts of several models would produce a more realistic model. Barber and Cushman (1981) and Riggan and Cole (1981) have recently developed two models for nitrogen uptake in land treatment for perennial forage grass and for forest systems respectively. The model by Barber and Cushman, based on Michaelis-Menten kinetics, can be represented by

$$J = \frac{J_{max}\, C_l}{K_m + C_l} - E \qquad (17)$$

where J is the flux, J_{max} is the maximum flux at high C_l, C_l is the concentration of the nutrient in the solution at the root/solution interface, K_m is the Michaelis-Menten constant, and E is the efflux. This model was tested in the laboratory and with corn field data and good agreement was obtained.

The computational model by Riggan and Cole (1981) has been shown to be useful in predicting forest production and nitrogen uptake by trees at a young Douglas fir experimental site.

Table 2. Main characteristics of the models* (from Frissel and van Veen 1981)

Processes	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)
Microbiological															
Urea → NH_4		x										x			
Minor./immob.	x		x		x	x	x	x	x	x	x		x		
Micro. biomass						x	x	x	x						
Nitrification			x	x	x	x			x						
Denitrification	x	x	x	x	x	x			x					x	x
Biol. N_2-fix									x						
Plant physiological															
Water uptake	x	x	x	x	x				x	x			x		
Dry matter prod.		x							x	x	x				
Root growth	x	x	x						x	x					
Debris, exudation									x						
N uptake	x	x	x	x	x			x	x	x			x		
Physical															
Water flux	x	x	x	x	x	*		*	*	x		x	x	x	
Heat flux		x			x	*									
Gas flux					x							x			
NH_4 ads/exch.	x	x	x	x		x		x	x	x		x		x	
NH_4-volatil.	x					x						x			
Leaching	x	x	x	x	x	x		x	x	x			x		

* Data on water flux and moisture content and/or heat flux are derived from another (external) simulation program.

1 (Tanji et al. 1981)
2 (Wagenet 1981)
3 (Rao et al. 1981)
4 (Selim & Iskandar 1981)
5 (Kruh & Segall 1981)
6 (Van Veen & Frissel 1981)
7 (Juma et al. 1981)
8 (Boxatta 1981)
9 (McGill et al. 1981)
10 (Seligman & Van Keulin 1981)
11 (Russell 1981)
12 (Parton et al. 1981)
13 (Addiscott 1981)
14 (Leffelaar 1981)
15 (Smith 1981)

Systematic comparison of nitrogen models

Frissel and van Veen (1981) systematically compared 15 nitrogen models (Table 2). These models vary widely in their purpose and the processes included. Models 1 - 5 are the most general ones, with the microbiological processes described by rather simple equations. Models 6 - 9 emphasize the role of microorganisms in mineralization-immobilization, and models 9 and 10 give special consideration to dry matter production. Model 11 concentrates on long-term prediction and models 12 - 15 are focused on one process only. Table 3 summarizes additional information on the models, including the main objective of the models, time horizon of interest, input data requirement, and type of equations used for model solving. This comparison between models is not conclusive since there are many other models that are not included, but it does point out the availability in the literature of many types of N models that can be used in land treatment.

The model by Selim and Iskandar (1978, 1980, 1981) has been developed for slow rate land treatment systems and has been evaluated using data from

Table 3. Additional characteristics of the models* (from Frissel and van Veen 1981)

Processes	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)
Main Objective															
Scientific understanding	x	x		x		x	x	x	x			x		x	x
Forecast					x						x		x		
Management			x							x					
Time horizon															
Days	x			x								x		x	x
Months		x	x	x	x	x	x		x	x			x		
Years						*		x			x				
Input data															
Climatic	x	x	x	x	x	x		x	x	x		x	x	x	
Soil physical	x	x	x	x	x	x		x	x	x		x	x	x	x
Soil biochemical	x	x	x	x	x	x	x	x	x	x	x				x
Soil microbiological						x	x	x	x						
Vertical distribution of parameters	x	x	x	x	x	x				x			x		x
Type of equations															
Partial differential	x	x		x	x							x		x	
Differential		x	x	x	x	x	x	x	x		x				x
Balance			x					x		x		x	x		x

*A very long-term version of the model exists but is not included.

1 (Tanji et al. 1981)
2 (Wagenet 1981)
3 (Rao et al. 1981)
4 (Selim & Iskandar 1981)
5 (Kruh & Segall 1981)
6 (van Veen & Frissel 1981)
7 (Juma et al. 1981)
8 (Bosatta 1981)
9 (McGill et al. 1981)
10 (Seligman & Van Keulin 1981)
11 (Russell 1981)
12 (Parton et al. 1981)
13 (Addiscott 1981)
14 (Leffelaar (1981)
15 (Smith 1981)

lysimeter studies (Iskandar and Selim 1981). Nakano et al. (1981) developed a nitrogen model for overland flow systems. Both models contain water flow and nitrogen transport and transformation submodels. Selim and Iskandar's (1981) model is one-dimensional under steady and transient conditions and is for two-dimensional flow. This model is flexible and valid for uniform as well as multilayered soils and can be used for 1) estimating the application rate and schedule of wastewater to land, 2) determining the fate of wastewater N species in soils, 3) predicting plant uptake of N, 4) predicting groundwater depth in land treatment, 5) estimating land area required to renovate wastewater, 6) estimating storage capacity, and 7) assisting managers and decision-makers in further simplification and adaptation for solving specific problems.

Selim and Iskandar (1981) tested their model for sensitivity to changes in the rate of nitrification, NH_4 exchange rate, and rate of plant

uptake of N. The model was further evaluated with controlled experiments using ^{15}N.

The model by Nakano et al. (1981) showed that, based on knowledge of water movement, the processes of N transport and transformation in overland flow (in order of importance) are adsorption of NH_4 by the soil surface, nitrification of NH_4, transport of NO_3 to the subsurface layers or runoff, and plant uptake of both NH_4 and NO_3.

All mechanistic N models such as those of Selim and Iskandar (1981) and Nakano et al. (1981) need further field evaluation, while conceptual and optimization models may be used at the present time. A typical useful conceptual N model is that described by Mehran et al. (1981).

MODELING PHOSPHORUS TRANSPORT AND TRANSFORMATION

Several models have been developed with a view to describing P movement in soils. These range in complexity and scope from rather simple, empirical models which may involve kinetics (Enfield 1974, Ryden and Pratt 1980) or may not (Taylor and Kunishi 1974, Harter and Foster 1976), to models based on sorption theory and kinetics (Enfield and Bledsoe 1975, Enfield and Shew 1975, Novak et al. 1975, Shah et al. 1975, Enfield et al. 1976, Mansell et al. 1977a, Selim 1978). In some cases, more complex, mechanistic multiphase models have been adopted in which the importance of kinetics is emphasized (Mansell et al. 1977b) or de-emphasized (Enfield et al. 1977). Some of these models (Enfield 1974, Enfield et al. 1976) are not concerned with P movement, per se, but with the kinetics of P sorption by soils, which is an important aspect of P movement. Enfield (1978) has reviewed several aspects of empirical sorption theory and mechanistic multiphase models for P movement in soils.

One of the simplest models proposed to date is that of Harter and Foster (1976). It involves an empirical polynomial sorption equation which expresses the relationship between the amount of P sorbed and that added in the form:

$$y = A + BX + CX^2 + DX^3 + EX^4 \qquad (18)$$

where Y is the amount of P sorbed and X the amount of P added. The major advantage of this model is its simplicity in that it does not require a complicated moisture movement computer program for water transport. This approach, however, ignores the kinetics of P sorption which has a varying effect depending on the soil in question (Ryden et al. 1977). The impor-

tance of including kinetics in empirical models has been emphasized by Enfield and Shew (1975), Enfield (1976) and Enfield et al. (1976). Furthermore, the Harter and Foster (1976) model was developed by using only one concentration of added P, and without the adoption of a generalized theory, the model requires a considerable amount of laboratory work to determine the parameters describing P sorption for each soil. In addition, there has been no evaluation of the effectiveness of the model. Nevertheless, this and similar empirical models have potential for predicting P movement in soil and require field evaluation.

The mechanistic multiphase model developed by Mansell et al. (1977b) attempts to describe a very much more complex system. Chemical kinetics and transport theory are used to describe the interaction and movement of P in soil. Four phases of soil P are assumed: physically adsorbed, chemisorbed, water-soluble, and precipitated. The kinetics of the reactions between any two of the four phases is considered to be reversible and six kinetic reactions are considered. This model almost certainly represents the first multiphase kinetic approach to simulate P movement. The model was used by Mansell et al. (1977b) to describe the transport of applied P during steady water flow for a range of rate coefficients. The equations used were as follows:

$$\frac{\partial(\theta A)}{\partial t} = -\theta\,(k_1 A^N + k_5 A) + \rho(k_2 B + k_6 D) \qquad (19)$$

$$\frac{\partial(\theta B)}{\partial t} = k_1 \theta A^N - (k_2 + k_3)\,\rho B + k_4 C \qquad (20)$$

$$\frac{\theta(\rho C)}{\theta t} = k_3 \rho B\; k_4 \rho C \qquad (21)$$

$$\frac{\partial(\rho D)}{\partial t} = k_5\,(\theta A) - k_6 \rho D \qquad (22)$$

where θ = volumetric soil water content

ρ = soil bulk density

t = time

A = concentration of P in solution

B = amount of P adsorbed

C = amount of P immobilized (chemisorbed)

D = amount of P precipitated

N = constant indicating order of the adsorption process

k_1 = rate coefficient for adsorption

k_2 = rate coefficient for desorption

k_3 = rate coefficient for immobilization

k_4 = rate coefficient for mobilization

k_5 = rate coefficient for precipitation

k_6 = rate coefficient for dissolution.

The complexity of multiple mechanistic and transport models, however, may pose limitations in that the models require the evaluation of numerous parameters relating to P sorption by the soil at the treatment site, as well as the measurement of a range of field variables. Consequently, a generally applicable and simple model is needed to predict P movement in soils which can be applied to existing or potential treatment areas that are unlikely to be intensively monitored.

Ryden and Pratt (1979) discussed a simple model for prediction of P removal from wastewater. This model is essentially that described in the Process Design Manual for Land Treatment of Municipal Wastewater (U.S. EPA et al. 1977) and has been recently evaluated by Ryden et al. (1981) using data from three existing land application sites. The model relies on the conformity of P sorption by soil at a specific treatment area to a generalized isotherm describing P soil sorption (Ryden and Syers 1977). Conformity of P sorption to this isotherm has been observed for a wide range of contrasting subsoils and topsoils (Ryden et al. 1977, Ryden and Syers 1977, Ryden and Pratt 1979).

The generalized isotherm describes the relationship between the fractional saturation (θ) of the P sorption maximum of the soil and the solution P concentration at equilibrium (Fig. 3). This isotherm provides a rather simple method of assessing equilibrium sorption capacity at a specified solution P concentration. The specified solution P concentration may be as high as that in the wastewater applied or as low as that regarded as being a maximum concentration in the applied effluent by a regulatory agency. From this estimate of P sorption capacity at the specified solution P concentration (in most cases the mean dissolved inorganic P concentration of the effluent applied), the longevity of the treatment area may be calculated from

$$T = \frac{S_p}{I_p - H_p} \qquad (23)$$

where

T = the time in years for the P to reach a given depth in the profile

S_p = the P storage capacity (kg/ha) of the volume of soil above that depth

I_p = the P input (kg/ha yr)

H_p = the amount of P removed in any harvested crop.

Equation 23 assumes that the net P input ($I_p - H_p$) reacts progressively with successive depth elements of the soil profile. The sorption capacity, as defined above, of the first depth element becomes saturated before appreciable amounts of P move into the next depth element. By implication, therefore, the boundary between P-enriched and nonenriched soil is assumed to be rather abrupt. The model also considers that water movement is unimportant relative to the kinetics of the P reactions and that time is sufficient for slow reactions to have an appreciable impact on the extent of P retention within the soil profile. Ryden et al. (1981) described a procedure for collecting data input to the model and the results of model evaluation using sites at CRREL in Hanover, New Hampshire, and at Fort Devens, Massachusetts. The New Hampshire results indicated that the P balance model predicted site longevity of approximately 50 and

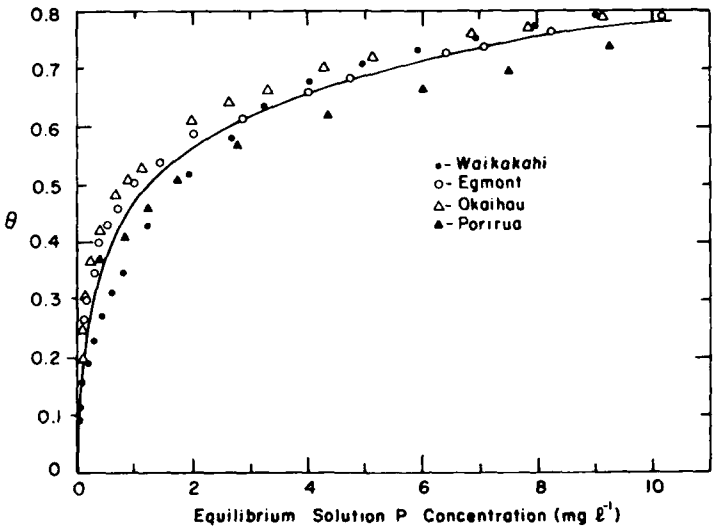

Figure 3. Generalized equilibrium isotherm for P sorption by soils where θ (the fractional saturation of the equilibrium sorption maximum) is plotted against the equilibrium solution P concentration (Ryden et al. 1981).

210 years for a Windsor sandy loam and a Charlton silt loam respectively. The existing depth of P enrichment in these profiles predicted from the model agreed closely with measurement of P enrichment based on amounts of NaOH, extractable P and on measured soil solution P concentrations. Approximately 85% of the P enrichment of the profile occurred within the predicted depth. For the third site (Ft. Devens, gravelly, sandy soil) estimates of site longevity indicated that the profile was saturated with respect to P removal (to a depth of 1.5 m). However, wastewater travels through several meters before it mixes with groundwater and further P removal occurs.

Ryden et al. (1981) concluded that the P model described above provides a simple and fairly reliable prediction of the P storage capacity of a soil profile used for land treatment of wastewater. From the P storage capacity value, site longevity can be estimated. In many practical situations an estimate of storage capacity and site longevity is all that is required during site evaluation with respect to P removal from wastewater. The P sorption model provides this information with a minimum of effort devoted to laboratory sorption studies. The model can also be used for site management during operation of land treatment. Data from soil analyses taken every few years, along with other model input (plant uptake and P applied), would provide information on the rate of P removal, the degree of soil saturation with respect to P, and concentration of P in renovated water. However, further field evaluation of this model is needed.

MODELING VIRUS MOVEMENT IN SOILS

The fate of pathogens that survive modern wastewater treatment is a major public health concern. These pathogens include enteric viruses, bacteria, parasitic helminths, and protozoa. Viruses may survive most modern wastewater treatment practices, including chlorination (Gerba et al. 1975). There has been little success in correlating virus fate with that of other reliable indicator organisms such as fecal coliforms (Mack et al. 1972, Bell 1976, Schaub and Sorber 1977), mainly due to differences in size.

Recently, Vilker (1981) reviewed the literature on virus removal by soils and soil materials, and he concluded that available data could be represented by either a Langmuir or a Freundlich isotherm. However, the equilibrium strongly favors the liquid phase over the adsorbed phase, which has important implications in laboratory column studies or field experiments.

Vilker and Burge (1980) recognized the need for a model to describe virus movement in soils that incorporates the effects of virus type, wastewater application rate and composition, frequency and amount of rainfall and soil composition. The objective of such an effort was to describe the breakthrough or concentration history of viruses in a soil bed effluent. They developed an adsorption-mass transfer model which involves diffusion of virus particles to the solid surface and the local hydrodynamic effects of the fluid phase near the surface. In this approach, the effects of changing soil water composition with depth were not included.

Vilker (1981) concluded that it is unlikely that movement of viruses through soils will be completely described by modeling. However, modeling, along with observation data, can provide a method for ranking soils according to their relative strength to detain and to permanently inactivate enteric viruses. The model described by Vilker and Burge (1980) and Vilker (1981) has provided useful information on the factors controlling virus movement in soils, and recommendations to enhance the removal of viruses by soils have been suggested.

Attempts to describe the fate of viruses in aerosols have been initiated (Sorber et al. 1976, Schaub et al. 1978, Kowel 1980). Viruses have been detected up to 100 m from the spray point, whereas bacteria were not detected in aerosols at distances of even 10 m from sprinklers.

MODELING TOXIC METALS AND TRACE ORGANIC MOVEMENT IN SOILS

A report was prepared by a group of 30 scientists (Council on Agricultural Science and Technology 1976) assessing the potential hazards of heavy metals and other elements in sewage sludge (which is also applicable to wastewater). Elements categorized as posing relatively little hazard include Mn, Fe, Al, Cr, As, Se, Sb, Pb and Hg. Those considered of potentially serious hazard in sludge and land application are Cd, Cu, Mo, Ni and Zn. Page et al. (1981) have recently discussed the effects of these metals on plant growth, uptake by crops and their behavior in soils.

Mathematical simulation models for trace element movement in soils have progressed slowly in accuracy during the past decade, but they are not advanced enough to be useful due to 1) inadequate characterization of the organic complexing agents in natural water and wastewater, 2) lack of knowledge on redox status of wastewater and soil solution, 3) inavailability of thermodynamic constant data, and 4) lack of kinetic data for

chemical and biological processes. Nevertheless several models have simulated trace element transport and transformation in soils. Sposito and Mattigod (1980) developed a mathematical model (GEOCHEM) for computing equilibrium speciation of chemical elements in soil solution.

Modeling trace organic movement in land treatment is just beginning to draw attention, mainly due to the lack of analytical methods for trace organic measurements and the presence of many types of organics in wastewater. The U.S. Environmental Protection Agency Laboratory, at Ada, Oklahoma, is currently developing and evaluating mathematical models to describe the fate of toxic organics in soils.

SUMMARY AND CONCLUSIONS

Significant progress has been made in developing mathematical and optimization models for land treatment planning, design and management. The models reviewed and discussed in this report vary in their objectives, complexity, method of solution, input/output parameters and degree of validation. In general, there are two types of models: 1) the management-oriented models and 2) the research-oriented models. The former models are simpler and can be used in decision-making. Efforts made in developing models of the latter type are progressing to improve our understanding of the complex interactions of wastewater constituents with soils, but the main difficulty is to overcome soil spatial variability and the lack of field data for validation. Nevertheless, several models have been field evaluated and can be used for land treatment planning, design and management.

RESEARCH NEEDS

The following are some of the topics for future research on modeling wastewater renovation using land treatment (Iskandar et al. 1981):

1. There is an urgent need to evaluate modeling efforts under field conditions.
2. Due to spatial variability in soil properties commonly encountered in the field, stochastic considerations need to be incorporated in deterministic models.
3. Improved in situ field instrumentation is needed to more precisely sample and measure water, solutes, and gases in land treatment systems.

4. More quantitative understanding is needed on the dynamics of water and nutrient absorption by plant roots.
5. Simulation of water and nutrient uptake by plants requires more data on root growth dynamics and activity under field conditions.
6. More emphasis should be placed on development and use of two-dimensional water- and solute-transport models.
7. More effort should be made to couple unsaturated flow models with saturated (groundwater) models, particularly in regard to the mixing phenomena at the interface.
8. Of the three modes of land application of liquid wastes, modeling of water and solute transport in overland flow systems needs the greatest attention.
9. There is a need for further development and testing of management-oriented models for planners, designers, and managers of land treatment systems.
10. Since most process modeling efforts cannot provide simulation for optimum solutions, there is a need for coupling these simulation models with optimization-type models.
11. The effects of environmental parameters and their interactions on model coefficients and constants need to be more comprehensively determined.
12. Field and laboratory experimentation is needed to determine and evaluate coefficients and constants in mathematical models under the prevailing environmental conditions.
13. There is a need to incorporate the carbon cycle in nitrogen transformation and transport modeling for better understanding of mineralization-immobilization and denitrification. The use of ^{15}N and ^{14}C tracers for better assessment of the rate and extent of N transformation processes is encouraged.
14. More quantitative determinations of denitrification and ammonia volatilization for the three modes of wastewater application are needed for improved predictions of gaseous losses of nitrogen.
15. There is a need to develop better methods for treating the dynamics of microbial populations and growth in land treatment systems.
16. Development and evaluation of models to describe the transport and transformations of trace organics, trace elements, viruses, and other pathogens in land treatment systems are needed.

17. The behavior of phosphorus, particularly organic P, in soils having differing chemical and mineralogical properties needs to be elucidated.

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